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PITTSBURGH ATOMIC SCIENCES INSTITUTE

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PROJECT SCIENTIST:	M. A. Biondi, Director Professor of Physics Telephone: Area Code 412 624-4354
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TITLE OF WORK:	ATOMIC AND MOLECULAR PROCESSES

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I. Experimental Investigations of Laser Processes

A. Electron-Ion Recombination under Laser Plasma Conditions (M. A. Biondi)

The 3-mode microwave afterglow apparatus and ultrahigh vacuum gas handling system was partially disassembled. Modifications were made to the vacuum system consisting of additional ultrahigh vacuum valves and stainless steel refrigerated traps to permit controlled vapor pressures of mercury and mercury compounds to be introduced to the quartz plasma-afterglow cylinder in the microwave cavity. In addition, desired amounts of noble gases (e.g. helium and xenon) can be introduced to the plasma region for control of electron heating/cooling rates and ion-molecule reaction paths.

Initial studies of mercury afterglows, with helium used as the inert buffer gas to control electron energy gain/loss rates and reduce ambipolar diffusion loss, were unsuccessful in achieving conditions where Hg_2^+ ions dominated the afterglow for the desired recombination studies. As a result, a more complex ion generation sequence, based on the ion-molecule reaction studies described in Sec. I.B, was used to make Hg_2^+ ions the principal afterglow ions. Xenon was added to the helium and mercury vapor, so that the ion generation/conversion sequence was $Xe^+ \rightarrow Xe_2^+ \rightarrow Hg^+ \rightarrow Hg\,Xe^+ \rightarrow Hg_2^+$.

At present, studies of the electron temperature (T_e) dependence of the recombination coefficient $\alpha(Hg_2^+)$ are in progress. The value at 300 K, $\alpha \sim 5 \times 10^{-7}$ cm^3/sec, agrees reasonably with earlier measurements at thermal energy. The excited state production by dissociative recombination is presently under investigation over the electron temperature range, 300 K < T_e < 10,000 K. One of the principal products of recombination over the whole electron temperature range is the 7^3S state, as evidenced by the 5461 Å radiation from the afterglow.

B. Ion-Molecule Reactions of Laser Interest (R. Johnsen)

The drift tube-mass spectrometer apparatus was modified to permit studies of ion-molecule reactions involving mercury or mercury compounds. Initially, the modified apparatus has been applied to studies of atomic and molecular rare gas ions with mercury atoms, usually via the additional residence time technique but in the case of the molecular ions by the change in arrival time spectra of the parent ions.

The results for the rare-gas atomic ions are summarized in Table I. Only

Table I. Rare-gas atomic-ion reactions with mercury at thermal energy

REACTION	RATE COEFFICIENT (cm^3/sec)
$He^+ + Hg \rightarrow He + Hg^+$	2.5 (-9)
$Ne^+ + Hg \rightarrow Ne + Hg^+$	< 5 (-13)
$Ar^+ + Hg \rightarrow Ar + Hg^+$	< 5 (-13)
$Kr^+ + Hg \rightarrow Kr + Hg^+$	< 1 (-12)
$Xe^+ + Hg \rightarrow Xe + Hg^+$	< 1 (-13)

the $He^+ + Hg$ reaction is fast; the others are undetectably slow.

The molecular rare-gas ion reactions with mercury are tabulated in Table II; two are undetectably slow.

Table II. Rare-gas molecular-ion reactions with mercury at thermal energy

REACTION	RATE COEFFICIENT (cm^3/sec)
$He_2^+ + Hg \rightarrow 2\ He + Hg^+$	4.5 (-10)
$Ne_2^+ + Hg \rightarrow 2\ Ne + Hg^+$	5 (-11)
$Ar_2^+ + Hg \rightarrow 2\ Ar + Hg^+$	< 1 (-12)
$Kr_2^+ + Hg \rightarrow 2\ Kr + Hg^+$	< 1 (-12)
$Xe_2^+ + Hg \rightarrow 2\ Xe + Hg^+$	5 (-10)

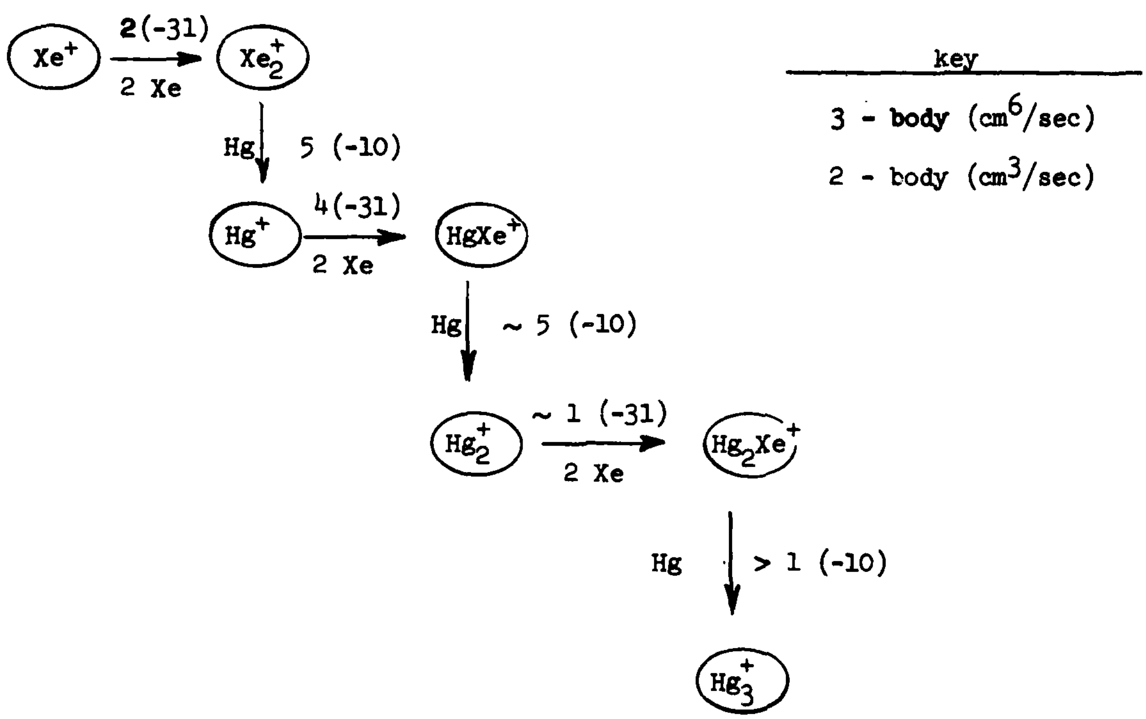
In addition, the reaction

$$Ar_2^+ + Xe \rightarrow Ar + Ar + Xe^+$$

proceeds with a rate coefficient $k \simeq 6 \times 10^{-10}$ cm^3/sec at 300 K.

The xenon-mercury reaction sequence leading to production of molecular ions of mercury is found to involve a combination of fast 2-body and moderately fast 3-body reactions, as indicated in Table/Figure III.

Table/Figure III. Xenon-mercury reactions



At present the reactions involving Hg Br_2 molecules are under study and preliminary rate coefficient values have been obtained. It is expected that final values will be obtained during the next report period.

III. Theoretical Investigations of Laser Processes

A. Ion-ion recombination (J. N. Bardsley)

Our basic computer program to evaluate the rate of ion-ion recombination at intermediate pressures is complete, and has been applied to rare-gas halide systems at several values of temperature and pressure.

We have confirmed our earlier speculation that an increase in the ambient temperature leads to a significant lowering of the recombination rate at low pressure but has little effect at high pressure. Due to these changes the peak in the recombination rate is pushed to higher pressure and is reduced in magnitude.

During this summer, in collaboration with B. Whitten of Miami University of Ohio, we began to investigate the dependence of the recombination rate upon the charge density by examining the effects of screening upon the recombining ion pair. The application of the Debye shielding theory suggests that this effect may lead to a reduction in the recombination rate for charge densities appropriate to high-power lasers or disturbed atmospheres.

Modelling calculations for rare-gas halide lasers, performed by L. Morgan at Livermore, suggest that the recombination rates may be significantly lower than those predicted by the chemical theories. We are planning to make one code available to them and to perform further analysis to check whether these preliminary results are consistent with our theory. This analysis will involve a more comprehensive study of screening effects.

B. Electron collisions with molecules (J. N. Bardsley)

We are adapting our resonance scattering code to permit us to make an analysis of dissociative attachment to $HC\ell$. Recent experimental results from Yale University suggest that the cross section may be very sensitive to the rotational and vibrational state of the $HC\ell$ molecule. The necessary modifications to the code have been completed but have not yet been fully tested. We are currently developing the theoretical model on which our computations will be based.

C. Ion-molecule reactions (J. N. Bardsley)

The analysis of the response of the atmosphere to intense beams requires an understanding of the rates, over a broad range of temperatures, for many ion-molecule reactions. As part of our collaboration with the NOAA Aeronomy Group at Boulder we have completed a study of charge transfer from O^- in collisions with O_2. This work has helped to resolve the large differences between beam measurements of this reaction rate.

IV. Publications and Technical Presentations

A. Publications

Resonant Contributions to Single Charge Transfer between He^{2+} and He, J. N. Bardsley, James S. Cohen and J. M. Wadehra, Phys. Rev. A 19, 2129 (1979).

Molecular Resonance Phenomena, J. N. Bardsley, In Electron-Molecule and Photon-Molecule Collisions, Eds. T. Rescigno, V. McKay and B. Schneider (Plenum, 1979), 267.

The Mobility of He^+ Ions in He, S. Sinha, S. L. Lin and J. N. Bardsley, J. Phys. B 12, 1613 (1979).

Cross Section for the Reaction $O^- + O_2 \rightarrow O_2^- + O$ at Relative Kinetic Energies 0.04 - 2 eV, S. L. Lin, J. N. Bardsley, I. Dotan, F. C. Fehsenfeld and D. L. Albritton, Int. J. Mass. Spectrom. Ion Phys., in press.

Thermal-Energy Charge Transfer, Quenching and Association Reactions of Doubly Charged Ions in the Rare Gases, Rainer Johnsen and Manfred A. Biondi, Phys. Rev. A 20, 87, 1979.

B. Technical Presentations

Cross Section for the Reaction $O^- + O_2 \rightarrow O_2^- + O$ at Relative Kinetic Energies 0.04-2 eV, presented by J. N. Bardsley at the Gaseous Electronics Conference, October 1979.

Charge-Transfer and Association Reactions Involving Mercury and Rare-Gas Ions, presented by R. Johnsen at the Gaseous Electronics Conference, October 1979.

V. Visiting Scientists

B. Whitten, Miami University of Ohio.

Senior Investigator	Est. Funds Expended and Committed (Thous.)
J. N. Bardsley	122.0
M. A. Biondi	230.0
W. L. Fite	56.7
F. Kaufman	147.4
E. C. Zipf	43.5
Total Expended and Committed	599.6
Available Funds	604.9
Estimated Funds Remaining as of 9/30/79	5.3

University Accounting of Funds

Expended as of 9/30/79	599.6
Available Funds	604.9
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